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A METHOD FOR EVALUATING MODEL PARAMETERS BY NUMERICAL INVERSION

By

Gary A. Ethridge

April 1971

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UNITED STATES ARMY ELECTRONICS COMMAND - FORT MONMOUTH, NEW JERSEY

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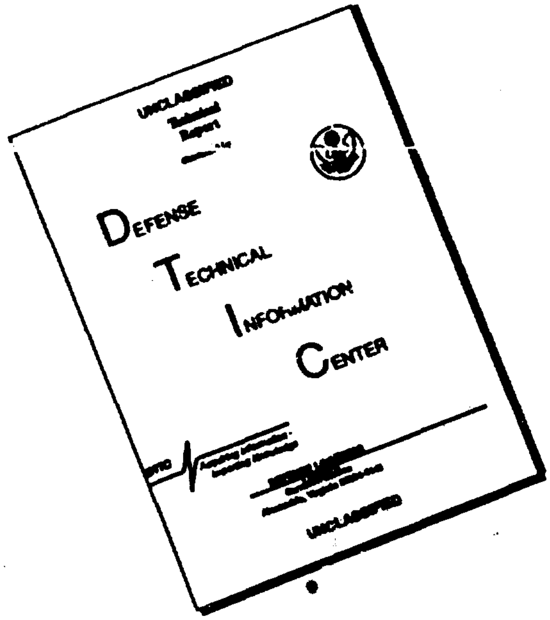

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INTRODUCTION

The solution to a mathematical theory may take a variety of forms including solutions which can be described in closed form or numerical solutions which require a complex digital computer program if closed form solutions cannot be derived. Regardless of the type of solution obtained, there are usually a number of unknowns or crudely estimated physical parameter values. In any case, some method of finding the set of parameter values is needed such that the model results will "best" fit observation. One technique for finding these "best" values is least-squares curve fitting. Closed form solutions can be fitted by one of several methods to give the best fit to the data by the least-squares criterion. Unlike the closed form type of solution, complex numerical solutions are not easily adapted to least-squares curve fitting.

In theory it should be possible to invert the model and use the data to evaluate the unknown parameter values. One simple method might be to run the computer program using different input parameters, observing the variation in the output so as to make a subjective estimate of the best values. Repeated trials could narrow down the range of values, but the expenditure of individual effort and costly computer time would be undesirable for other than the simplest models.

This report describes a technique which determines the "best" parameter values, in a least-squares sense, for a computer simulation of a complex physical process by using the program, field data, and a variation of the differential corrections least-squares curve-fitting method.

THEORY

Suppose that a model of an observed natural phenomenon exists and that to be able to rely fully upon the results that the model can supply, several parameters require numerical estimates. One way to determine the best values for these empirical constants is to take data of the physical process, invert the model solution, and solve for the unknown parameters. Where complications arise in the execution of this method, least-squares curve fitting can be used to recover the parameter values which give the "best" estimates in a least-squares sense.

With data in the form (x_i, y_i), $i = 1,2,3, \ldots N$, one selects a model, i.e., a function $F(x; a_1, a_2, \ldots a_M)$ of x and M undetermined parameters a_j, $j = 1,2,3, \ldots M$ such that $F(x_i; a_1, a_2, \ldots a_M)$ will best fit the data points y_i, $i = 1,2,3 \ldots N$. The "best" set of values for the a_j, $j = 1,2, \ldots M$, in a least-squares sense will be found when the sum of the squares of the differences in the functional evaluation of x_i and y_i is a minimum over all the data points (x_i, y_i), $i = 1, 2, \ldots N$. That is

$$\sum_{i=1}^{N} [F(x_i; a_1, a_2, \ldots a_M) - y_i]^2$$

is a minimum. Most methods of least-squares curve fitting will specify the form of F which is to be used as the model. The curve-fitting technique of differential corrections [1-3] requires no special form for the model function $F(x_i; a_1, a_2, \ldots a_M)$. Restrictions on the properties of F are:

1) F must be a single-valued function of x and of the M parameters a_j.

2) F must be differentiable with respect to the M parameters a_j.

Because differential corrections technique does not specify the form of the function F to be used, F may assume the form of a sequence of operations in a digital computer program. Most computer numerical solutions to equations describing a physical process behave as functions in that there exists an independent variable, say x, such that the numerical solution given by the digital computer program can be regarded as a single-valued function of x, and the dependent variable(s) will usually be differentiable in one or more model parameters. It should then be possible to use a computer program as a function F in such a way that the methods of least-squares curve fitting can be applied to F. This report describes a method of accomplishing this, saving the excessive labor and costly computer time involved in a trial-and-error approach.

The method of differential corrections and its application to the least-squares curve fitting of a computerized mathematical model solution will be discussed below.

Given the set of data points (x_i, y_i) $i = 1,2,3, \ldots N$, let the difference between the function value $F(x_i; a_1, a_2, \ldots a_M)$ and the data point y_i be called the residual v_i where

$$v_i = F(x_i; a_1, a_2, \ldots a_M) - y_i. \qquad (1)$$

A best fit by the least-squares criterion will be obtained when the undetermined values a_j, $j = 1,2, \ldots M$, give a minimum for

$$\sum_{i=1}^{N} v_i^{\,2}.$$

The values for the a_j's can be found by the solution of the following set of simultaneous equations:

$$\frac{\partial}{\partial a_1} \sum_{i=1}^{N} v_i^{\,2} = 0,$$

$$\frac{\partial}{\partial a_2} \sum_{i=1}^{N} v_i^{\,2} = 0, \qquad \ldots, \tag{2}$$

$$\frac{\partial}{\partial a_M} \sum_{i=1}^{N} v_i^{\,2} = 0.$$

When F is represented by a digital computer program, the equations cannot be solved directly, and an iterative scheme must be used.

Let $a_j = a_j^o + \Delta a_j$ where the superscript o refers to first approximations so that the Δa_j's are the corrections needed to force $\Sigma v_i^{\,2}$ to a minimum. Writing equation (1) with $F(x;\ a_1^o + \Delta a_1,\ a_2^o + \Delta a_2,\ \ldots\ a_M^o + \Delta a_M)$ expanded in a Taylor series, we have

$$v_i = F(x_i;\ a_1^o,\ a_2^o,\ \ldots a_M^o) + \Delta a_1 \frac{\partial F_i}{\partial a_1^o} + \Delta a_2 \frac{\partial F_i}{\partial a_2^o}$$

$$+ \Delta a_3 \frac{\partial F_i}{\partial a_3^o} + \ldots + \Delta a_M \frac{\partial F_i}{\partial a_M^o} - y_i + \text{(higher order terms)}. \tag{3}$$

Assuming a sufficiently close estimate on the initial approximations a_i^o, the higher order terms will be neglected. Defining R_i as the residual $R_i = y_i - F_i^o$ where $F_i^o = F(x_i;\ a_1^o,\ a_2^o,\ \ldots\ a_M^o)$ equation (3) can be written

$$v_i = \Delta a_1 \frac{\partial F_i}{\partial a_1^o} + \Delta a_2 \frac{\partial F_i}{\partial a_2^o} + \Delta a_3 \frac{\partial F_i}{\partial a_3^o} + \ldots + \Delta a_M \frac{\partial F_i}{\partial a_M^o} - R_i. \tag{4}$$

The system of equations (2) which are to be solved give for the [illegible] equation

$$\sum_i \left(\Delta a_1 \frac{\partial F_i}{\partial a_1^o} + \Delta a_2 \frac{\partial F_i}{\partial a_2^o} + \ldots + \Delta a_M \frac{\partial F_i}{\partial a_M^o} - R_i\right) \frac{\partial F_i}{\partial a_j^o} = 0.$$

Letting

$$A_{j,k} = \sum_i \frac{\partial F_i}{\partial a_j^o} \frac{\partial F_i}{\partial a_k^o}$$

and

$$B_j = \sum_i R_i \frac{\partial F_i}{\partial a_j^o},$$

we have the algebraic system of simultaneous equations (2) written in matrix form

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots & A_{1M} \\ A_{21} & A_{22} & A_{23} & \cdots & A_{2M} \\ \cdot & & & & \\ \cdot & & & & \\ \cdot & & & & \\ A_{M1} & A_{M2} & A_{M3} & \cdots & A_{MM} \end{pmatrix} \begin{pmatrix} \Delta a_1 \\ \Delta a_2 \\ \cdot \\ \cdot \\ \cdot \\ \Delta a_M \end{pmatrix} = \begin{pmatrix} B_1 \\ B_2 \\ \\ \\ \\ B_M \end{pmatrix} \qquad (5)$$

Since $A_{j,k} = A_{k,j}$ the matrix system above is symmetric allowing only the evaluation of the upper triangle and making use of the square-root method for solving symmetric systems of simultaneous equations [1,4,5].

Having obtained the corrections Δa_j, $j = 1,2,3, \ldots M$, they either satisfy the least-squares requirement when added to a_j^o, giving the $a_j = a_j^o + \Delta a_j$, or the newly formed a_j's give a new set of first approximations say b_j, and a new set of corrections Δb_j is evaluated. Convergence for the method may be said to have been reached when no significant change in the set of model parameters a_j, $j = 1,2, \ldots M$ is exhibited; that is, when

$$\sum_{j=1}^{M} \Delta a_j^2 \leq \varepsilon,$$

for $\varepsilon > 0$, results from cycle to cycle.

To apply the method of differential corrections curve fitting to a computerized numerical solution, one must use a numerical approximation for each of the required partial derivatives

$$\frac{\partial F_i}{\partial a_j^o}$$

as defined above. Use is made of a seven-point numerical formula described below [6].

Given discrete points (a_i, F_i) of a tabulated function $F_i = F(a_i)$ for $i = -J, -(J-1), \ldots -1, 0, 1, 2, \ldots J$ for equispaced points a_i with $a_{i+1} - a_i = h$, the first derivative

$$\frac{dF}{da} = F'$$

evaluated at a_o is given as follows:

$$F'_o = \frac{1}{2h}\left[F_1 - F_{-1} - \frac{1}{6}(\delta^2 F_1 - \delta^2 F_{-1}) + \frac{1}{30}(\delta^4 F_1 - \delta^4 F_{-1})\right]$$

with $\delta F_i = F_{i+1/2} - F_{i-1/2}$. This gives the formula

$$\begin{aligned} F'_o = [F_1 - F_{-1} &- 1/6(F_2 - 2F_1 + 2F_{-1} - F_{-2}) \\ &+ \frac{1}{30}(F_3 - F_2 - 3(F_2 - F_1) + 3(F_1 - F_o) - F_o + F_{-1}) \\ &- \frac{1}{30}(F_1 - F_o - 3(F_o - F_{-1}) + 3(F_{-1} - F_{-2}) - F_{-2} + F_{-3})]. \end{aligned}$$

Use of this algorithm gives the required partial derivatives for the differential corrections method described above. However, one may improve on the evaluation of partial derivatives in the event that one or more of the model parameters a_j are used in a subfunction f of the numerical routine. When these individual functions f (i.e., one of the governing equations in the mathematical formulation of the problem) can be defined, it is recommended that the chain rule for calculating derivatives be used. Letting F be the main program solution and f an intermediate solution, a subprogram, or the like, then

$$\frac{\partial F_i}{\partial a_j} = \frac{\partial F_i}{\partial f}\frac{\partial f}{\partial a_j}.$$

This rule can provide better convergence in the routine described above.

EXAMPLES

Atmospheric Diffusion

An atmospheric diffusion model for the prediction of contaminant concentrations in the atmosphere will be treated with the curve-fitting technique previously described. The concentration C is a function of downwind travel distance x and several atmospheric parameters, together with empirically determined constants. The mathematical theory used is based upon the application of the similarity theory [7,8] of the surface boundary layer as related to diffusion in the atmosphere [9].

The concentration function $C(x;\, a_1,\, a_2,\, a_3,\, a_4)$ is given by

$$C = \frac{QK}{L^2 u_*} \, \frac{1}{\zeta^2 (f(\zeta) - f(\zeta_o))}$$

where

$$\frac{dx}{dt} = \frac{u_*}{k} (f(\zeta) - f(\zeta_o)),$$

$$\frac{d\zeta}{dt} = b u_* \, \emptyset(\zeta),$$

$$\emptyset(\zeta) = \left(1 - \left|\frac{df}{d\zeta}\right|^{-1}\right)^{1/4},$$

$$f(\zeta) = \ln(c\zeta/\zeta_o) + \beta(\zeta - \zeta_o)$$

where the sumbols are defined as follows:

Q = source strength

L = atmospheric parameter

u_* = atmospheric parameter

k = Kármán's constant

b = empirical constant

c = empirical constant

x = downwind travel distance of substance

$\zeta = \frac{z}{L}$

z = vertical height coordinate

t = time.

These representative equations for modeling atmospheric diffusion using similarity theory have been solved numerically using a digital computer. The curve-fitting technique previously described will be tested by evaluating the empirical constants c and β, and also by inserting into the $\emptyset$ function two parameters to be fitted, α_1 and α_2, given by

$$\emptyset(\zeta) = (\alpha_1 - \left(\frac{df}{d\zeta}\right)^{-1})^{\alpha_2}.$$

Original specifications for the α's are $\alpha_1 = 1$ and $\alpha_2 = 1/4$.

For this example, a test case was developed by specifying c, β, α_1, and α_2 to generate a sample data deck. Then, approximations to c, β, α_1, and α_2 are given, and by using the data the original parameters will be recovered.

First only c and β are evaluated as shown in Table 1-A. Then c, β, α_1, and α_2 are evaluated together as given in Table 1-B. The results of the test case show how model parameters for atmospheric diffusion theories can be evaluated using field data and the curve-fitting technique described herein.

A Ballistic Missile

The curve-fitting technique was applied to the problem of determining the drag coefficient of a ballistic missile using radar position data of the missile during flight [1]. To use the data in a curve fit of the type described, an accurate realistic model of the trajectory during all phases of the missile's performance is required.

The ballistic model selected is a five-degree-of-freedom ballistic missile trajectory and impact prediction digital computer program, TRAJ [10], used for missile flight safety at White Sands Missile Range, and also utilized in studies of meteorological effects on a ballistic missile by the Atmospheric Sciences Laboratory. Only the three position coordinates relative to the launcher will be used in the test case. Hence, X, Y, Z are the dependent variables*, and Mach number, m,

---

*Differential corrections method applied to a vector-valued function is described in Appendix A.

TABLE I-A

CURVE FIT FOR c AND β

INITIAL ESTIMATES: $c^{\circ} = 1.$, $\beta^{\circ} = 5.$

ITERATION STEP	1	2	3	4	5	6	7
CORRECTIONS							
Δc	.498313	-.091784	-.006609	.000081	-.000001	0.	0.
$\Delta\beta$	-5.39567	.497557	-.089023	-.013029	.000133	.000013	-.000001
NEW ESTIMATES							
c°	.501686	.59347	.600079	.599999	.600000	.600000	.600000
β°	10.39567	9.898120	9.987143	10.000172	10.00004	10.000027	10.000028
ABSOLUTE ERROR							
$\sum_i \lvert R_i \rvert$	21.97333	8.17993	.682987	.099759	.0973442	.097336	.0973336

Convergence attained at step 7 given by $\sum_i |\Delta c_i| \leq .00001$

Actual test case values $c = 0.6$, $\beta = 10.0$

Final residual $R = .0973339$

TABLE I-B

CURVE FIT FOR c, β, α_1, α_2

INITIAL ESTIMATES: $c = .5$, $\beta = 8.$, $\alpha_1 = 1.5$, $\alpha_2 = .3$

ITERATION STEP	1	2	3	4	5	6	7	8
CORRECTIONS								
Δc	.431388	-.109547	.065436	.013314	-.000430	-.000159	-.000003	0.
$\Delta\beta$	-1.207020	-1.276570	1.134080	-.695554	.034183	.010550	.000308	.000012
$\Delta\alpha_1$	.722685	-.244213	.008445	.011892	.001217	-.000029	.000002	0.
$\Delta\alpha_2$	-.062313	-.057175	.142239	.024320	.002797	.000108	.000024	0.
NEW ESTIMATES								
c^o	.568612	.678159	.612722	.599408	.599838	.5999997	.600000	.600000
β	9.207020	10.483590	9.349510	10.045064	10.010880	10.000330	10.000022	10.000010
α_1^o	.777315	1.021528	1.013082	1.001191	.9999973	1.000002	1.000000	1.000000
α_2^o	.362313	.419488	.277249	.252929	.250132	.250024	.250001	.250001
ABSOLUTE ERROR								
$\sum_i \lvert\Delta_i\rvert$	33.272	49.050	3.870	.954	.220	.0992	.0974	.0973

Convergence attained at step 8 given by $\sum_i |\Delta c_i| \leq .0001$

Actual test case values $c = .6$, $\beta = 10.$, $\alpha_1 = 1.$, $\alpha_2 = .25$

Final residual $R = .097338$

will be assumed to be the only independent variable of the model. Although there are many input parameters to TRAJ, only the aerodynamic coefficients of the drag curve will be considered as influences on the missile's trajectory.

A test case was generated by using a known drag curve as input and putting the (x, y, z) output on data cards. The input drag curve was constructed to give the characteristic shape and values of an actual drag curve, although most drag curves are provided in the form of a table. Nevertheless one could "piecewise" fit for a drag function if no single expression can be used. Hence the drag curve used is

$$C_d = (\alpha_1 + \alpha_2 x + \alpha_3 (m + .8)^5) \, \mathrm{Exp}(- \frac{(m+1)^4}{10})$$

where initially values for α_1, α_2, and α_3 are .25, .5, and .75, respectively. Results of the iteration process are given in Table II. The first approximations were specified and the original values of the parameters were obtained, to a certain degree of accuracy.

SUMMARY

This report describes a method of curve fitting for a broad class of functions not representable by simple terms in a closed-form expression. These functions can assume the identity of complex sequences of operations in a digital computer program and yet have suitable properties for curve fitting. This technique will afford considerably more flexibility to the engineer or scientist who wishes to curve fit a function to field data without overly simplifying the function to be used. The investigator can now build a complex, sophisticated mathematical model of a physical process, solve the equations numerically on a digital computer and use field data and the method described here to find unknown parameters of the physical system.

TABLE II

CURVE FIT FOR α_1, α_2, α_3

INITIAL ESTIMATES: $\alpha_1 = .2$, $\alpha_2 = .55$, $\alpha_3 = .8$

[illegible]	2	4	6	8	10	15	19	23
[illegible]	[illegible]	[illegible]	.0060191	-.0029464	.0022839	-.0006035	-.0012429	.0001487
[illegible]	[illegible]	[illegible]	-.0305403	.0077066	.0011545	.0014603	.0029398	-.0004515
[illegible]	[illegible]	[illegible]	.034442	.0002690	[illegible]	-.0000121	-.0001244	.0000206
[illegible]	[illegible]	[illegible]	[illegible]	.2523615	[illegible]	.2494799	.2494665	[illegible]
[illegible]	[illegible]	[illegible]	.4728545	.4707785	[illegible]	.4967600	.4980020	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	.7506302	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	13.067	13.914
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

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APPENDIX A

Suppose data have been observed in which there exists more than one dependent variable for a common independent variable. Then the data will be of the form $(x_i, \hat{Y}_i)$ where $\hat{Y}_i$ is a vector of L components. Let $\hat{F}(x_i; a_1, a_2, \ldots a_M)$ be a vector-valued function of L components which is to approximate the $\hat{Y}_i$ in a least-squares sense. The problem is to find the best set of a_j's, $j = 1, 2, \ldots M$ such that

$$\sum_{i=1}^{N} (\hat{F}_i - \hat{Y}_i) \cdot (\hat{F} - \hat{Y}_i)$$

is a minimum, where the dot (•) represents the scalar product of two vectors. Let the vector of differences $\hat{V}_i$ be

$$\text{A1)} \qquad \hat{V}_i = \hat{F}_i - \hat{Y}_i .$$

Setting $a_j = a_j^{\circ} + \Delta a_j$ and expanding (A1) in Taylor series

$$\hat{V}_i = \hat{F}(x_i; a_1^{\circ}, a_2^{\circ}, \ldots a_M^{\circ}) + \Delta a_1 \frac{\partial \hat{F}_i}{\partial a_1^{\circ}} + \Delta a_2 \frac{\partial \hat{F}_i}{\partial a_2^{\circ}} + \ldots$$

$$+ \Delta a_M \frac{\partial \hat{F}_i}{\partial a_M^{\circ}} + (\text{higher order terms}) - \hat{Y}_i .$$

If $\hat{R}_i = \hat{Y}_i - \hat{F}_i^{\circ}$ where $\hat{F}_i^{\circ} = \hat{F}(x_i; a_1^{\circ}, a_2^{\circ}, \ldots a_M^{\circ})$ then

$$\hat{V}_i = \Delta a_1 \frac{\partial \hat{F}_i}{\partial a_1^{\circ}} + \Delta a_2 \frac{\partial \hat{F}_i}{\partial a_2^{\circ}} + \ldots + \Delta a_M \frac{\partial \hat{F}_i}{\partial a_M^{\circ}} - \hat{R}_i .$$

The condition for $\Sigma \hat{V}_i \cdot \hat{V}_i$ to be a minimum is that

$$\frac{\partial}{\partial \Delta a_j} (\Sigma \hat{V}_i \cdot \hat{V}_i) = 0$$

[illegible], $\ldots M$. The equations [illegible]

$$\frac{\partial \hat{V}_i}{\partial \Delta a_j} \cdot \hat{V} \quad [illegible], \ldots$$

This gives for each j the equation

$$\sum_{i=1}^{N} \left(\Delta a_1 \frac{\partial \hat{F}_i}{\partial a_1^o} + \Delta a_2 \frac{\partial \hat{F}_i}{\partial a_2^o} + \ldots + \Delta a_M \frac{\partial \hat{F}_i}{\partial a_M^o} - \hat{R}_i\right) \cdot \frac{\partial \hat{F}_i}{\partial a_j^o} = 0.$$

Letting

$$A_{j,k} = \sum_{i=1}^{N} \frac{\partial \hat{F}_i}{\partial a_j^o} \cdot \frac{\partial \hat{F}_i}{\partial a_k^o}$$

and

$$B_j = \Sigma \hat{R}_i \cdot \frac{\partial \hat{F}_i}{\partial a_j^o}$$

then the system of equations in matrix form is

$$\text{A3)} \qquad \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1M} \\ A_{21} & A_{22} & \cdots & A_{2M} \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ A_{M1} & A_{M2} & \cdots & A_{MM} \end{pmatrix} \cdot \begin{pmatrix} \Delta a_1 \\ \Delta a_2 \\ \cdot \\ \cdot \\ \cdot \\ \Delta a_M \end{pmatrix} = \begin{pmatrix} B_1 \\ B_2 \\ \cdot \\ \cdot \\ \cdot \\ B_M \end{pmatrix}$$

the solution of which is identical to the solution given in the text.

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